High-Precision Arithmetic and Mathematical Physics

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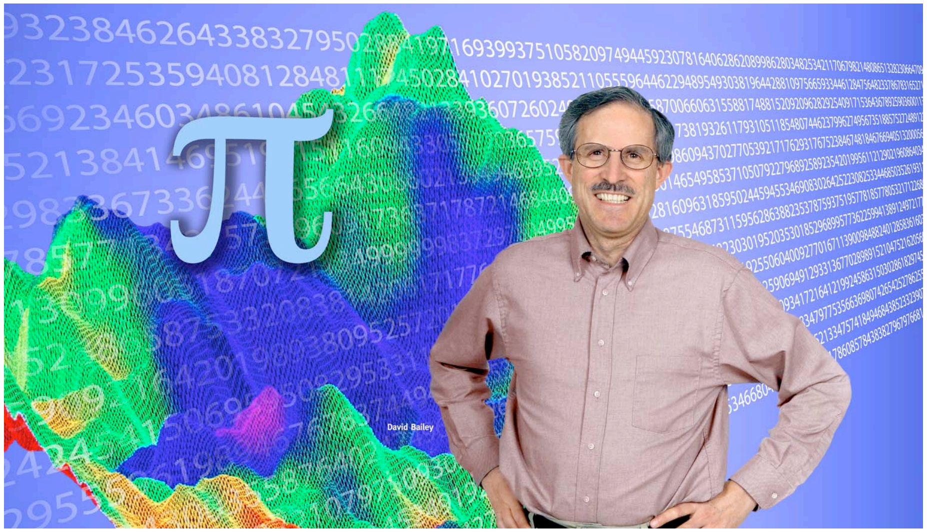


Applications of High-Precision Arithmetic in Modern Scientific Computing

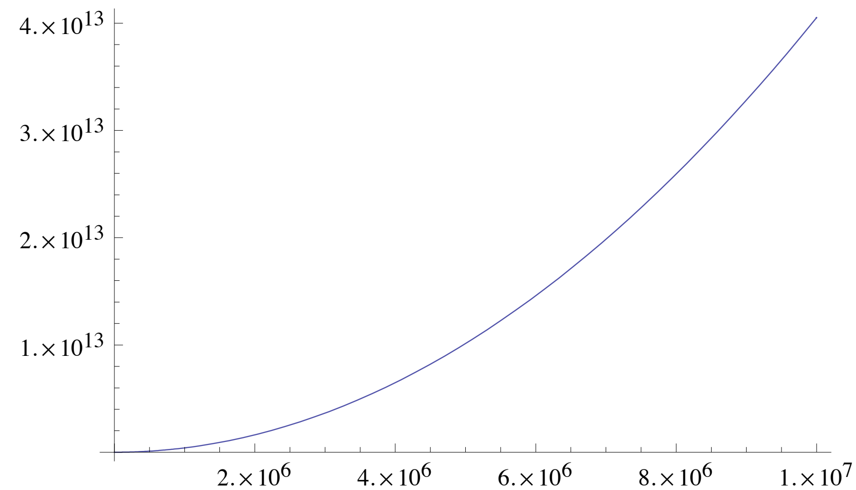
- Highly nonlinear computations.
- Computations involving highly ill-conditioned linear systems.
- Computations involving data with very large dynamic range.
- Large computations on highly parallel computer systems.
- Computations where numerical sensitivity is not currently a major problem, but periodic testing is needed to ensure that results are reliable.
- Research problems in mathematics and mathematical physics that involve constant recognition and integer relation detection.

Few physicists, chemists or engineers are highly expert in numerical analysis. Thus high-precision arithmetic is often a better remedy for severe numerical round-off error, even if the error could, in principle, be improved with more advanced algorithms or coding techniques.

Growth of Condition Number with System Size

Consider the very simple differential equation y''(x) = -f(x). Discretization leads to the matrix:

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{bmatrix}$$



The condition number of this matrix (the quotient of the largest eigenvalue to the smallest eigenvalue) is readily seen to be approximately

$$\kappa(n) \approx \frac{4(n+1)^2}{\pi^2}$$

For modest-sized n (relative to many huge systems now being attempted), systems of this type cannot be reliably solved using 64-bit arithmetic.

Available High-Precision Facilities

Vendor-supported arithmetic:

Type	Total Bits	Significant Digits	Support
IEEE Double	64	16	In hardware on almost all systems.
IEEE Extended	80	18	In hardware on Intel and AMD systems.
IEEE Quad	128	33	In software from some vendors (50-100X slower than IEEE double).

Non-commercial (free) software:

Type	Total Bits	Significant Digits	Support
Double-double	128	32	DDFUN90, QD.
Quad-double	256	64	QD.
Arbitrary	Any	Any	ARPREC, MPFUN90, GMP, MPFR.

Commercial software: *Mathematica, Maple*.

LBNL's High-Precision Software

- QD: double-double (31 digits) and quad-double (62 digits).
- ARPREC: arbitrary precision.
- Low-level routines written in C++.
- C++ and Fortran-90 translation modules permit use with existing C++ and Fortran-90 programs -- only minor code changes are required.
- Includes many common functions: sqrt, cos, exp, gamma, etc.
- PSLQ, root finding, numerical integration.

Available at: **http://www.experimentalmath.info**

Authors: Xiaoye Li, Yozo Hida, Brandon Thompson and DHB

GMP and MPFR

GNU Multiprecision Library:

- High-level signed integer arithmetic functions (mpz).
- High-level rational arithmetic functions (mpq).
- High-level floating-point arithmetic functions (mpf).
- C++ class-based interface to all of the above.

Available at: http://gmplib.org/

MPFR:

- C library of floating-point accurately rounding arithmetic functions.

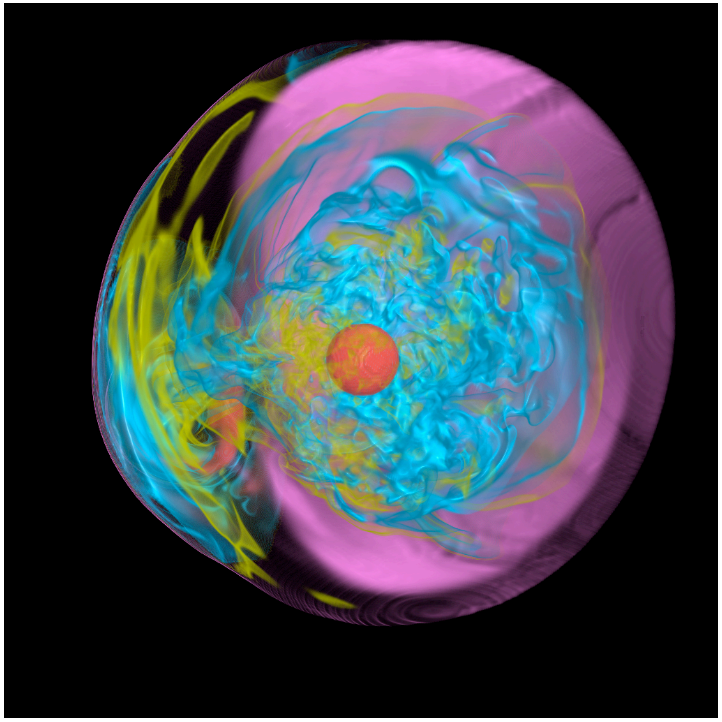
Available at: http://www.mpfr.org

C++ high-level interfaces based on MPFR:

- MPFRCPP
- MPFR++
- GMPFRXX

Application of High-Precision Arithmetic: Supernova Simulations

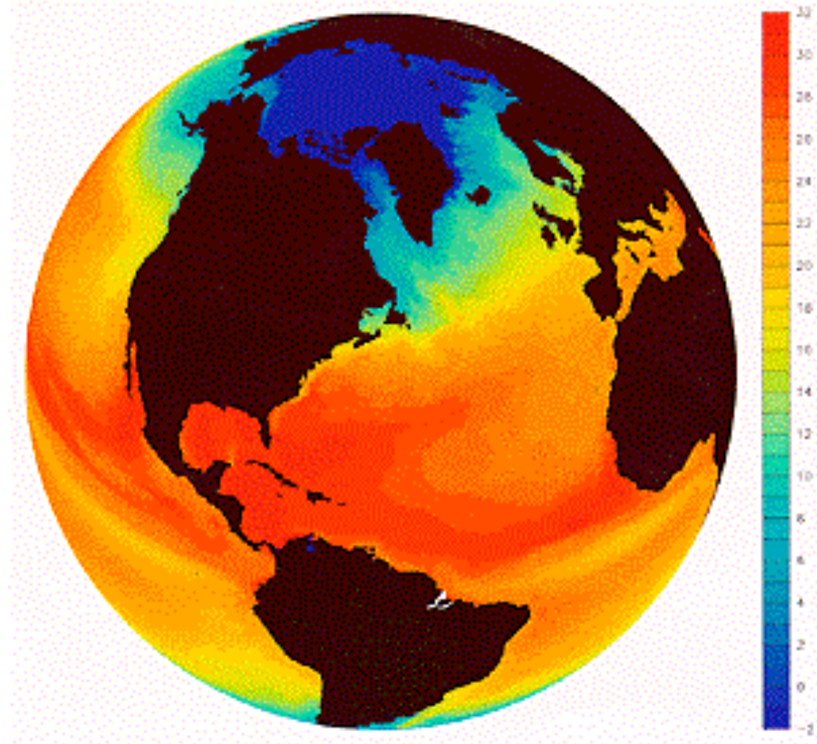
- Researchers at LBNL are using QD to solve for non-local thermodynamic equilibrium populations of iron and other atoms in the atmospheres of supernovas.
- Iron may exist in several species, so it is necessary to solve for all species simultaneously.
- Since the relative population of any state from the dominant state is proportional to the exponential of the ionization energy, the dynamic range of these values can be very large.
- The quad-double portion now dominates the entire computation.



P. H. Hauschildt and E. Baron, "The Numerical Solution of the Expanding Stellar Atmosphere Problem," *Journal Computational and Applied Mathematics*, vol. 109 (1999), pg. 41-63.

Climate Modeling

- Climate and weather simulations are fundamentally chaotic – if microscopic changes are made to the current state, soon the future state is quite different.
- In practice, computational results are altered even if minor changes are made to the code or the system.
- This numerical variation is a major nuisance for code maintenance.
- He and Ding of LBNL found that by using double-double arithmetic to implement a key inner product loop, most of this numerical variation disappeared.



Yun He and Chris Ding, “Using Accurate Arithmetics to Improve Numerical Reproducibility and Stability in Parallel Applications,” *Journal of Supercomputing*, vol. 18, no. 3 (Mar 2001), pg. 259-277.

Planetary Orbit Calculations

- A key question of planetary theory is whether the solar system is stable over cosmological time frames (billions of years).
- Scientists have studied this question by performing very long-term simulations of planetary motions.
- This problem is well known to exhibit chaos.
- Simulations typically do well for long periods of time, but then fail at certain key junctures, unless special measures are taken.
- Researchers have found that double-double or quad-double arithmetic is required to avoid severe numerical inaccuracies, even if other techniques are employed.

"The orbit of any one planet depends on the combined motions of all the planets, not to mention the actions of all these on each other. To consider simultaneously all these causes of motion and to define these motions by exact laws allowing of convenient calculation exceeds, unless I am mistaken, the forces of the entire human intellect." [Isaac Newton, 1687]

G. Lake, T. Quinn and D. C. Richardson, "From Sir Isaac to the Sloan Survey: Calculating the Structure and Chaos Due to Gravity in the Universe," *Proceedings of the Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, SIAM, Philadelphia, 1997, pg. 1-10.

Coulomb N-Body Atomic System Simulations

- Alexei Frolov of Queen's University in Canada has used MPFUN90 to solve a generalized eigenvalue problem that arises in Coulomb n-body interactions.
- Matrices are typically 5,000 x 5,000 and are very nearly singular.
- Frolov has also computed elements of the Hamiltonian matrix and the overlap matrix in four- and five-body systems.
- These computations typically require 120-digit arithmetic.

"We can consider and solve the bound state few-body problems which have been beyond our imagination even four years ago." – Frolov

A. M. Frolov and DHB, "Highly Accurate Evaluation of the Few-Body Auxiliary Functions and Four-Body Integrals," *Journal of Physics B*, vol. 36, no. 9 (14 May 2003), pg. 1857-1867.

Schrodinger Solutions for Lithium and Helium Atoms

- Zong-Chao Yan and colleagues at the University of Windsor have used high-precision arithmetic to obtain accurate solutions to the Schrodinger equation for the lithium atom.
- The ground state energy has now been calculated to an accuracy of a few parts in a trillion, a 1500X improvement over the best previous results.
- With these results, Yan and his colleagues have been able to test the relativistic and QED effects at the 50 parts per million level and also at the one part per million level.
- In related computations, high-precision arithmetic has been used in some theoretical calculations of the fine structure splittings in helium atoms. Experimental tests are now planned.

Z.-C. Yan and G. W. F. Drake, "Bethe Logarithm and QED Shift for Lithium," *Physics Review Letters*, vol. 81 (12 Sep 2003), pg. 774-777.

Electromagnetic Scattering Theory

- A key operation in computational electromagnetic scattering is to find the branch points of the asymptotic expansion of the spheroidal wave function.
- Schemes based on Newton-Raphson iterations using standard machine precision have accuracy limitations.
- The MPFUN90 package has been used to greatly extend the range of wavefunctions that can be studied with these simulations.
- This project required the conversion of a large body of existing Fortran code.

B. E. Barrowes, K. O'Neill, T. M. Grzegorczyk and J. A. Kong, "Asymptotic Expansions of the Prolate Angular Spheroidal Wave Function for Complex Size Parameter," *Studies in Applied Mathematics*, vol. 113 (2004), pg. 271-301.

The PSLQ Integer Relation Algorithm

Let (x_n) be a given vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$$

(or within "epsilon" of zero, where epsilon = 10^{-p} and p is the precision).

At the present time the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm. It was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

PSLQ (or any other integer relation scheme) requires very high precision (at least n*d digits, where d is the size in digits of the largest a_k), both in the input data and in the operation of the algorithm.

1. H. R. P. Ferguson, DHB and S. Arno, "Analysis of PSLQ, An Integer Relation Finding Algorithm," *Mathematics of Computation*, vol. 68, no. 225 (Jan 1999), pg. 351-369.
2. DHB and D. J. Broadhurst, "Parallel Integer Relation Detection: Techniques and Applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), pg. 1719-1736.

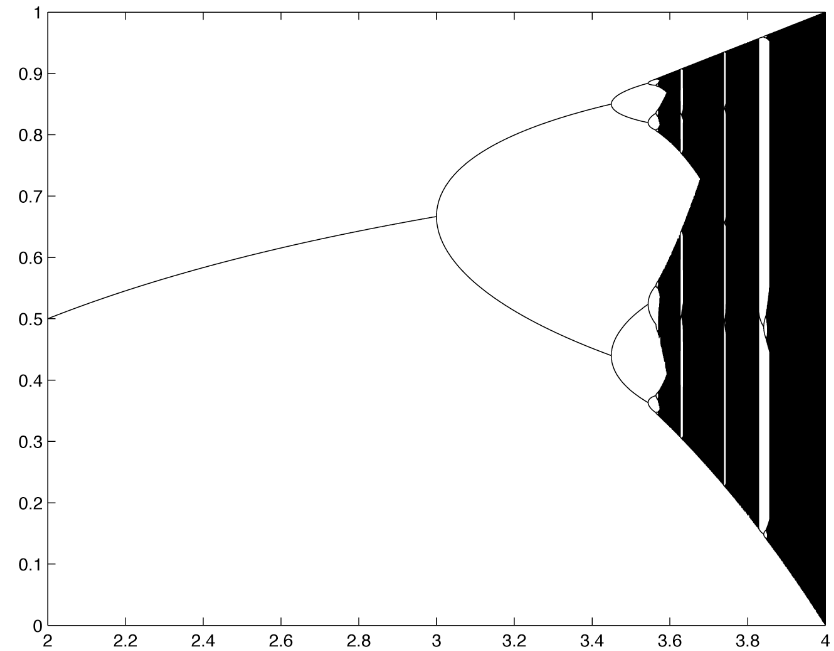
Bifurcation Points in Chaos Theory

Let t = B_3 = the smallest r such that the "logistic iteration"

$$x_{n+1} = rx_n(1 - x_n)$$

exhibits 8-way periodicity instead of 4-way periodicity.

By means of a sequential approximation scheme, one can obtain the numerical value of t to any desired precision:



3.544090359551922853615965986604804540583099845444573675457 81…

Applying PSLQ to (1, t, t^2, t^3, …, t^{12}), we obtained the result that t is a root of the polynomial:

$$\begin{aligned} 0 &= 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 \\ &\quad -193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12} \end{aligned}$$

The BBP Formula for Pi

In 1996, at the suggestion of Peter Borwein, Simon Plouffe used DHB's PSLQ program and arbitrary precision software to discover this new formula for pi:

$$\pi = \sum_{n=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

This formula permits one to compute binary (or hexadecimal) digits of pi beginning at an arbitrary starting position, using a very simple scheme that can run on any system with standard 64-bit or 128-bit arithmetic.

Recently it was proven that no base-n formulas of this type exist for pi, except $n = 2^m$.

1. DHB, P. B. Borwein and S. Plouffe, "On the Rapid Computation of Various Polylogarithmic Constants," *Mathematics of Computation*, vol. 66, no. 218 (Apr 1997), pg. 903-913.
2. J. M. Borwein, W. F. Galway and D. Borwein, "Finding and Excluding b-ary Machin-Type BBP Formulae," *Canadian Journal of Mathematics*, vol. 56 (2004), pg 1339-1342.

The Quinn-Rand-Strogatz Constant of Nonlinear Physics

Quinn, Rand, and Strogatz recently described a nonlinear oscillator system by means of the formula

$$0 = \sum_{i=1}^{N} \left(2\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2} - \frac{1}{\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2}} \right)$$

For large N, s = 1 – c / N (approx), where c = 0.6054436... Strogatz asked us to validate and extend this computation, and challenged us to identify this limit if it exists.

By means of a Richardson extrapolation scheme, implemented on 64-CPUs of a highly parallel computer system, we computed (using the QD software)

c = 0.60544365719673274947892284244720747522089960…

This led to the provable conclusion that the limit c exists and is the root of a Hurwitz zeta function (below). As a bonus, we obtained some asymptotic terms.

$$\zeta(1/2, x/2) = 0$$

DHB, J. M. Borwein and R. E. Crandall, “Resolution of the Quinn-Rand-Strogatz Constant of Nonlinear Physics,” *Experimental Mathematics*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/QRS.pdf.

Tanh-Sinh Quadrature

Given f(x) defined on (-1,1), define g(t) = tanh (pi/2 sinh t). Then setting x = g(t) yields

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;\approx\; h \sum_{j=-N}^{N} w_j f(x_j),$$

where x_j = g(hj) and w_j = g'(hj). Since g'(t) goes to zero very rapidly for large t, the product f(g(t)) g'(t) typically is a nice bell-shaped function for which the Euler-Maclaurin formula implies that the simple summation above is remarkably accurate. Reducing h by half typically doubles the number of correct digits.

Tanh-sinh quadrature is the best integration scheme for functions with vertical derivatives or blow-up singularities at endpoints, or for any function at very high precision (> 1000 digits).

1. DHB, Xiaoye S. Li and Karthik Jeyabalan, "A Comparison of Three High-Precision Quadrature Schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.
2. H. Takahasi and M. Mori, "Double Exponential Formulas for Numerical Integration," Publications of RIMS, Kyoto University, vol. 9 (1974), pg. 721–741.

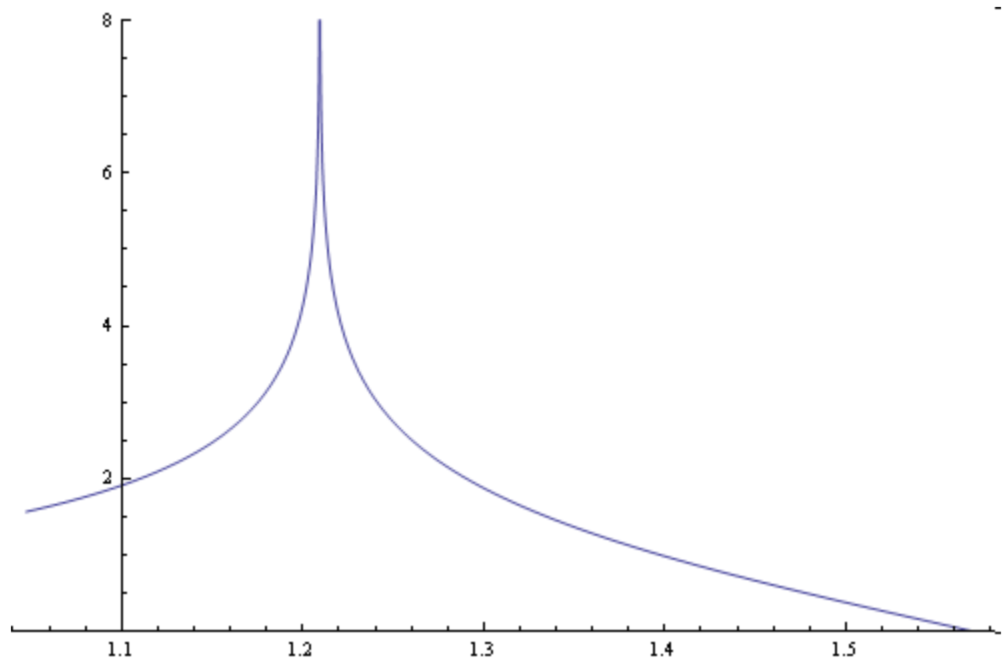
A Log-Tan Integral Identity

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| \mathrm{d}t \quad = \quad L_{-7}(2) \quad =$$

$$\sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This identity arises from analysis of volumes of knot complements in hyperbolic space. This is simplest of 998 related identities.

We have verified this numerically to 20,000 digits (using highly parallel tanh-sinh quadrature).



DHB, J. M. Borwein, V. Kapoor and E. Weisstein, "Ten Problems in Experimental Mathematics," *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481-409 .

Ising Integrals

We recently applied our methods to study three classes of integrals that arise in the Ising theory of mathematical physics – D_n and two others:

$$C_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i - u_j}{u_i + u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$E_n = 2\int_0^1 \cdots \int_0^1 \left(\prod_{1\le j<k\le n} \frac{u_k - u_j}{u_k + u_j}\right)^2 dt_2\, dt_3 \cdots dt_n$$

where in the last line $u_k = t_1\, t_2 \ldots t_k$.

DHB, J. M. Borwein and R. E. Crandall, "Integrals of the Ising Class," *Journal of Physics A: Mathematical and General*, vol. 39 (2006), pg. 12271-12302.

Computing and Evaluating C_n

We observed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

$$C_n = \frac{2^n}{n!} \int_0^\infty t K_0^n(t)\,\mathrm{d}t$$

where K_0 is the modified Bessel function. In this form, the C_n constants appear naturally in in quantum field theory (QFT).

We used this formula to compute 1000-digit numerical values of various C_n, from which the following results and others were found, then proven:

$$\begin{aligned}
C_1 &= 2 \\
C_2 &= 1 \\
C_3 &= \mathrm{L}_{-3}(2) = \sum_{n\geq 0}\left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2}\right) \\
C_4 &= \frac{7}{12}\zeta(3)
\end{aligned}$$

Limiting Value of C_n

The C_n numerical values appear to approach a limit. For instance,

$$C_{1024} = 0.63047350337438679612204019271087890435458707871273234\ldots$$

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC):
http://ddrive.cs.dal.ca/~isc

The result was:

$$\lim_{n\to\infty} C_n \quad = \quad 2e^{-2\gamma}$$

where gamma denotes Euler's constant. Finding this limit led us to the asymptotic expansion and made it clear that the integral representation of C_n is fundamental.

Other Ising Integral Evaluations

$$
\begin{aligned}
D_2 &= 1/3 \\
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2) \\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \\
E_2 &= 6 - 8\log 2 \\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 \\
&\quad + 16\pi^2\log 2 - 22\pi^2/3 \\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 \\
&\quad + 40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 \\
&\quad + 464\log^2 2 - 40\log 2
\end{aligned}
$$

where $\mathrm{Li}_n(x)$ is the polylog function. D_2, D_3 and D_4 were originally provided to us by mathematical physicist Craig Tracy, who hoped that our tools could help identify D_5.

The Ising Integral E_5

We were able to reduce E_5, which is a 5-D integral, to an extremely complicated 3-D integral.

We computed this integral to 250-digit precision, using a highly parallel, high-precision 3-D quadrature program. Then we used a PSLQ program to discover the evaluation given on the previous page.

We also computed D_5 to 500 digits, but were unable to identify it. The digits are available if anyone wishes to further explore this question.

$$
\begin{aligned}
E_5 \;=\; & \int_0^1 \int_0^1 \int_0^1 [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \\
& (-[4(x+1)(xy+1)\log(2)\,(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z\,((y^2+1)\,z^2 + 4(y+ \\
& 1)z+5)\,x^5 + y^2\,(4y(y+1)z^3 + 3\,(y^2+1)\,z^2 + 4(y+1)z - 1)\,x^4 + y\,(z\,(z^2+4z \\
& +5)\,y^2 + 4\,(z^2+1)\,y + 5z + 4)\,x^3 + ((-3z^2-4z+1)\,y^2 - 4zy + 1)\,x^2 - (y(5z+4) \\
& +4)x - 1)]\,/\,[(x-1)^3(xy-1)^3(xyz-1)^3] + [3(y-1)^2y^4(z-1)^2z^2(yz \\
& -1)^2x^6 + 2y^3z\,(3(z-1)^2z^3y^5 + z^2\,(5z^3+3z^2+3z+5)\,y^4 + (z-1)^2z \\
& (5z^2+16z+5)\,y^3 + (3z^5+3z^4-22z^3-22z^2+3z+3)\,y^2 + 3\,(-2z^4+z^3+2 \\
& z^2+z-2)\,y + 3z^3+5z^2+5z+3)\,x^5 + y^2\,(7(z-1)^2z^4y^6 - 2z^3\,(z^3+15z^2 \\
& +15z+1)\,y^5 + 2z^2\,(-21z^4+6z^3+14z^2+6z-21)\,y^4 - 2z\,(z^5-6z^4-27z^3 \\
& -27z^2-6z+1)\,y^3 + (7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)\,y^2 - 2\,(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)\,y + 7z^4-2z^3-42z^2-2z+7)\,x^4 - 2y\,(z^3\,(z^3 \\
& -9z^2-9z+1)\,y^6 + z^2\,(7z^4-14z^3-18z^2-14z+7)\,y^5 + z\,(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)\,y^4 + (z^6-14z^5+3z^4+84z^3+3z^2-14z+1)\,y^3 - 3\,(3z^5 \\
& +6z^4-z^3-z^2+6z+3)\,y^2 - (9z^4+14z^3-14z^2+14z+9)\,y + z^3+7z^2+7z \\
& +1)\,x^3 + (z^2\,(11z^4+6z^3-66z^2+6z+11)\,y^6 + 2z\,(5z^5+13z^4-2z^3-2z^2 \\
& +13z+5)\,y^5 + (11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)\,y^4 + (6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)\,y^3 - 2\,(33z^4+2z^3-22z^2+2z+33)\,y^2 + (6z^3+26 \\
& z^2+26z+6)\,y + 11z^2+10z+11)\,x^2 - 2\,(z^2\,(5z^3+3z^2+3z+5)\,y^5 + z\,(22z^4 \\
& +5z^3-22z^2+5z+22)\,y^4 + (5z^5+5z^4-26z^3-26z^2+5z+5)\,y^3 + (3z^4- \\
& 22z^3-26z^2-22z+3)\,y^2 + (3z^3+5z^2+5z+3)\,y + 5z^2+22z+5)\,x + 15z^2+2z \\
& +2y(z-1)^2(z+1) + 2y^3(z-1)^2z(z+1) + y^4z^2\,(15z^2+2z+15) + y^2\,(15z^4 \\
& -2z^3-90z^2-2z+15) + 15]\,/\,[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2] - [4(x+1)(y+1)(yz+1)\,(-z^2y^4 + 4z(z+1)y^3 + (z^2+1)\,y^2 \\
& -4(z+1)y + 4x\,(y^2-1)\,(y^2z^2-1) + x^2\,(z^2y^4 - 4z(z+1)y^3 - (z^2+1)\,y^2 \\
& +4(z+1)y+1) - 1)\log(x+1)]\,/\,[(x-1)^3x(y-1)^3(yz-1)^3] - [4(y+1)(xy \\
& +1)(z+1)\,(x^2\,(z^2-4z-1)\,y^4 + 4x(x+1)\,(z^2-1)\,y^3 - (x^2+1)\,(z^2-4z-1) \\
& y^2 - 4(x+1)\,(z^2-1)\,y + z^2-4z-1)\log(xy+1)]\,/\,[x(y-1)^3y(xy-1)^3(z- \\
& 1)^3] - [4(z+1)(yz+1)\,(x^3y^5z^7 + x^2y^4(4x(y+1)+5)z^6 - xy^3\,((y^2+ \\
& 1)\,x^2 - 4(y+1)x - 3)\,z^5 - y^2\,(4y(y+1)x^3 + 5\,(y^2+1)\,x^2 + 4(y+1)x + 1)\,z^4 + \\
& y\,(y^2x^3 - 4y(y+1)x^2 - 3\,(y^2+1)\,x - 4(y+1))\,z^3 + (5x^2y^2 + y^2 + 4x(y+1) \\
& y+1)\,z^2 + ((3x+4)y+4)z - 1)\log(xyz+1)]\,/\,[xy(z-1)^3z(yz-1)^3(xyz-1)^3])] \\
& /\,[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2]\; dx\,dy\,dz
\end{aligned}
$$

Recursions in Ising Integrals

Consider the 2-parameter class of Ising integrals (which arises in QFT for odd k):

$$C_{n,k} = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^{k+1}} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

After computing 1000-digit numerical values for all n up to 36 and all k up to 75 (performed on a highly parallel computer system), we discovered (using PSLQ) linear relations in the rows of this array. For example, when n = 3:

$$\begin{aligned}
0 &= C_{3,0} - 84C_{3,2} + 216C_{3,4} \\
0 &= 2C_{3,1} - 69C_{3,3} + 135C_{3,5} \\
0 &= C_{3,2} - 24C_{3,4} + 40C_{3,6} \\
0 &= 32C_{3,3} - 630C_{3,5} + 945C_{3,7} \\
0 &= 125C_{3,4} - 2172C_{3,6} + 3024C_{3,8}
\end{aligned}$$

Similar, but more complicated, recursions have been found for all n.

DHB, D. Borwein, J. M. Borwein and R. Crandall, "Hypergeometric Forms for Ising-Class Integrals," *Experimental Mathematics*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/meijer/pdf.

J. M. Borwein and B. Salvy, "A Proof of a Recursion for Bessel Moments," *Experimental Mathematics*, vol. 17 (2008), pg. 223-230.

Four Hypergeometric Evaluations

$$
\begin{aligned}
c_{3,0} &= \frac{3\Gamma^6(1/3)}{32\pi 2^{2/3}} = \frac{\sqrt{3}\pi^3}{8}\,{}_3F_2\left(\begin{array}{c}1/2, 1/2, 1/2\\ 1, 1\end{array}\middle|\frac{1}{4}\right)\\
c_{3,2} &= \frac{\sqrt{3}\pi^3}{288}\,{}_3F_2\left(\begin{array}{c}1/2, 1/2, 1/2\\ 2, 2\end{array}\middle|\frac{1}{4}\right)\\
c_{4,0} &= \frac{\pi^4}{4}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}^4}{4^{4n}} = \frac{\pi^4}{4}\,{}_4F_3\left(\begin{array}{c}1/2, 1/2, 1/2, 1/2\\ 1, 1, 1\end{array}\middle|1\right)\\
c_{4,2} &= \frac{\pi^4}{64}\left[4\,{}_4F_3\left(\begin{array}{c}1/2, 1/2, 1/2, 1/2\\ 1, 1, 1\end{array}\middle|1\right)\right.\\
&\quad \left.-3\,{}_4F_3\left(\begin{array}{c}1/2, 1/2, 1/2, 1/2\\ 2, 1, 1\end{array}\middle|1\right)\right] - \frac{3\pi^2}{16}
\end{aligned}
$$

DHB, J. M. Borwein, D. Broadhurst and M. L. Glasser, “Elliptic Integral Evaluations of Bessel Moments,” *Journal of Physics A: Mathematical and General*, vol. 41 (2008), pg 205203.

2-D Integral in Bessel Moment Study

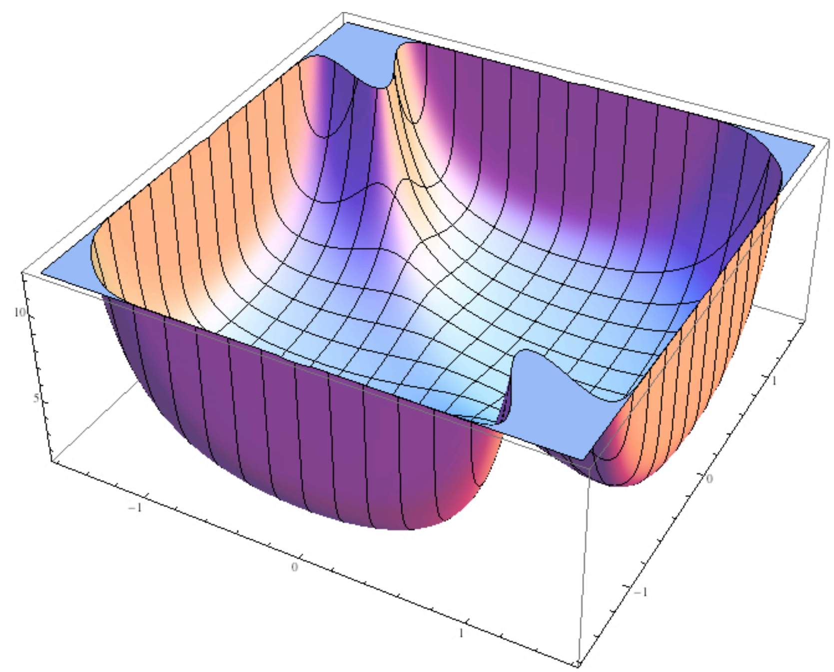
We conjectured (and later proved)

$$c_{5,0} \quad = \quad \frac{\pi}{2}\int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi + 4\sin^2(\theta+\phi)}}\,\mathrm{d}\theta\,\mathrm{d}\phi$$

Here **K** denotes the complete elliptic integral of the first kind

Note that the integrand function has singularities on all four sides of the region of integration.

We were able to evaluate this integral to 120-digit accuracy, using 1024 cores of the "Franklin" Cray XT4 system at LBNL.



Heisenberg Spin Integrals

In another recent application of these methods, we investigated the following "spin integrals," which arise from studies in mathematical physics:

$$P(n) \quad := \quad \frac{\pi^{n(n+1)/2}}{(2\pi i)^n} \cdot \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)$$
$$\times\, T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)\, \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n$$

where

$$U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \;=\; \frac{\prod_{1 \le k < j \le n} \sinh[\pi(x_j - x_k)]}{\prod_{1 \le j \le n} i^n \cosh^n(\pi x_j)}$$

$$T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \;=\; \frac{\prod_{1 \le j \le n} (x_j - i/2)^{j-1} (x_j + i/2)^{n-j}}{\prod_{1 \le k < j \le n} (x_j - x_k - i)}$$

H. E. Boos, V. E. Korepin, Y. Nishiyama and M. Shiroishi, "Quantum Correlations and Number Theory," *Journal of Physics A: Mathematical and General*, vol. 35 (2002), pg. 4443.

Evaluations of P(n)
Derived Analytically, Confirmed Numerically

$$P(1) = \frac{1}{2}, \quad P(2) = \frac{1}{3} - \frac{1}{3}\log 2, \quad P(3) = \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3)$$

$$P(4) = \frac{1}{5} - 2\log 2 + \frac{173}{60}\zeta(3) - \frac{11}{6}\zeta(3)\log 2 - \frac{51}{80}\zeta^2(3) - \frac{55}{24}\zeta(5) + \frac{85}{24}\zeta(5)\log 2$$

$$\begin{aligned} P(5) = {} & \frac{1}{6} - \frac{10}{3}\log 2 + \frac{281}{24}\zeta(3) - \frac{45}{2}\zeta(3)\log 2 - \frac{489}{16}\zeta^2(3) - \frac{6775}{192}\zeta(5) \\ & + \frac{1225}{6}\zeta(5)\log 2 - \frac{425}{64}\zeta(3)\zeta(5) - \frac{12125}{256}\zeta^2(5) + \frac{6223}{256}\zeta(7) \\ & - \frac{11515}{64}\zeta(7)\log 2 + \frac{42777}{512}\zeta(3)\zeta(7) \end{aligned}$$

and a much more complicated expression for P(6). Run times increase very rapidly with the dimension n:

n	Digits	Processors	Run Time
2	120	1	10 sec.
3	120	8	55 min.
4	60	64	27 min.
5	30	256	39 min.
6	6	256	59 hrs.

High-precision Arithmetic is Indispensible in Modern Scientific Computing

- State-of-the-art large-scale scientific calculations involving highly nonlinear systems often require numerical precision beyond conventional 64-bit floating-point arithmetic.
- Few physicists, chemists and engineers are experts in numerical analysis, so software-based high-precision arithmetic is often the best remedy for severe numerical round-off error.
- The emerging “experimental” methodology in mathematics and mathematical physics often requires hundreds or even thousands of digits of precision.
- Double-double, quad-double and arbitrary precision software libraries are now widely available (and in most cases are free).
- High-level C, C++ and Fortran-90 interfaces facilitate the conversion of large scientific programs to use this software.
- There is a critical need to develop much faster techniques for numerical integration in multiple dimensions.